THE
ICE INSTITUTE
PAMPHLET

ol. XXXII October, 1945 No. 4

Published by
THE RICE INSTITUTE

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THE RICE INSTITUTE PAMPHLET

Vol. XXXII October, 1945 No. 4

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THE APPLICATION OF GROUP THEORY TO THE NORMAL VIBRATIONS OF A CUBIC CRYSTAL*

ABSTRACT

THE use that can be made of group theoretical considerations in analyzing the normal vibrations of a crystal is illustrated in the case of a simple cubic lattice. The group under which the system is invariant can be made finite by the use of periodic boundary conditions. The invariant sub-group containing the translations only can be completely reduced on the basis of plane waves of arbitrary polarization. These can be divided into sets of 144 members, and each set gives rise to a representation of the whole group of the crystal. In a number of special cases these representations can be reduced with respect to various sub-groups of rotations to such an extent that it is possible to determine the directions of the normal vibrations. In such cases the frequencies can be directly expressed in terms of the force constants.

The group theoretical treatment makes it easy to distinguish those properties of the elastic spectrum which depend only on the symmetry of the lattice, from those which depend on special properties of the force constants.

* * *

The principal applications of group theory to mathematical physics are based on the invariance of the differential equations of physics to groups of transformations. The various solutions of the equations can be used as the elements

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on which a representation of the group can be based, and from the properties of the group and the theory of group representations, it is possible to draw some conclusions concerning the solutions themselves. I propose to illustrate here this use of group theory by considering in some detail its application to the problem of the normal vibrations of a simple cubic crystal lattice.

The problem of normal vibrations is of physical importance in a number of ways. It provides the basis for computation of the specific heat of the crystal, and for the effect of temperature on x-ray diffraction. It is also of importance in the theory of the electrical conductivity of metals and in the theory of residual rays. The first approach to such problems was made by Debye in 1913, when he developed his theory of specific heats. In this work he ignored all of the characteristically crystalline properties of the solid and treated it as an elastic continuum. About the same time Born and von Karman showed how the matter could be treated in terms of normal vibrations, and recently the application of group theory has made it possible to draw some general conclusions concerning the elastic spectrum of a crystal with a minimum of calculation. Although these conclusions give one a good view of the general situation, they usually fall just short of giving all of the information which is desired and need to be supplemented by some numerical calculation. Several years ago P. C. Fine, at the California Institute of Technology, carried through a numerical evaluation of the frequencies of the normal vibrations of a body-centered cubic crystal. As far as I know this is the first time that such a calculation has been carried to an explicit conclusion, and it provides an interesting example of a frequency distribution. However, the methods which I shall describe here are based on the group theoretical work of

Wigner,[1] Seitz,[2] and others, and lead to only those results that can be obtained from the symmetry of the problem and are independent of the nature of the forces.

THE NORMAL VIBRATIONS

For purposes of illustration, and to avoid complications, consider a simple cubic lattice. In its equilibrium configuration, this consists of a particle of mass m at every point whose coordinates, in a Cartesian system, are integers. The masses are connected together in such a way that the force acting on one of them is a linear function of the displacements of all of the points, itself included. If $\mathbf{r}_{l,m,n}$ is the displacement from its equilibrium position of the particle whose rest position has the coordinates (l,m,n), then the differential equations of motion are

$$m\frac{d^2\mathbf{r}_{l,m,n}}{dt^2}=\sum_{\lambda,\mu,\nu} A^{l,m,n}_{\lambda,\mu,\nu}\,\mathbf{r}_{\lambda,\mu,\nu} \tag{1}$$

The constants $A^{l,m,n}_{\lambda,\mu,\nu}$ depend only on $(l-\lambda)$, $(m-\mu)$, $(n-\nu)$, and get smaller as $(l-\lambda)^2+(m-\mu)^2+(n-\nu)^2$ increases. In order to avoid complications due to the boundaries, it is customary to apply cyclic boundary conditions. By these it is required that

$$\mathbf{r}_{l,m,n}=\mathbf{r}_{l+aG,m+bG,n+cG} \tag{2}$$

where G is a large integer that determines the size of the cycle, and a, b, and c are arbitrary integers. This type of boundary condition eliminates immediately all phenomena connected with the crystal surfaces. A model such as this will describe only pure volume phenomena, but it is believed

[1] E. Wigner, "Gruppentheorie," Vieweg u. Sohn.

[2] F. Seitz, "A Matrix-algebraic Development of the Crystallographic Groups," *Zs. f. Kristallographie*, vol. 88, p. 433, 1934; vol. 90, p. 289, 1935; vol. 91, p. 336, 1936; vol. 92, p. 100, 1937. F. Seitz, "On the Reduction of Space Groups," *Annals of Mathematics*, vol. 37, p. 17, 1936.

to include all of the elements essential to a discussion of the normal vibrations. Since it is linear, this model does not provide for the treatment of thermal conductivity or thermal expansion. These phenomena are associated with departures from linearity in the differential equations of motion. The boundary conditions reduce the number of effectively different lattice points to G^3, and G must be taken so large that the results are essentially independent of its size.

The existence of normal coordinates for a set of equations of this form is given by the general theory. These coordinates are linear combinations of the displacements,

$$\rho_s = \sum C^s_{l,m,n}\, r_{l,m,n} \tag{3}$$

such that

$$\frac{d^2\rho_s}{dt^2} = -\omega_s^2\, \rho_s^2 \tag{4}$$

The solution of these equations can be written down at once, and then by inversion of equations (3)

$$r_{l,m,n} = \sum D^{l,m,n}_s\, \rho_s \tag{5}$$

This gives the final solution of the problem. The principal point is then actually to find the normal coordinates, and the various coefficients $C^s_{l,m,n}$. By the application of group theoretical considerations this can be reduced to the solution of a cubic equation, when the lattice is simple cubic, and to an equation of order equal to three times the number of masses in a unit cell for other kinds. In special cases these equations can be further reduced by additional considerations based on the rotational symmetries of the crystal. This is the object of the group theoretical discussion given here.

The differential equations (1), and consequently (4), are invariant to any translation or rotation of the crystal lattice

at transforms the various equilibrium positions into themlves. The content of this statement is simply that the coficients $A^{l,m,n}_{\lambda,\mu,\nu}$ depend only upon the differences of the inces. The translations are

$$l \to l+a, \qquad m \to m+b, \qquad n \to n+c. \qquad T_t$$

he rotations are, for the simple cubic lattice, the members f the rotation group O to which a simple cube is invariant. he differential equation is also invariant under the inverion, or reflection through the origin, in which $l \to -l$, $m \to -m$, $\to -n$. The normal coordinates ρ_s constitute a basis for he establishment of a representation of this whole group ecause the differential equation for a normal vibration is nvariant under all these transformations. Furthermore, ince each differential equation for a normal vibration inludes only one frequency, the effect of any of the transfornations of this group will be to transform one normal vibraion to another, or linear combination of others, which ibrates with the same frequency. Hence those normal viorations whose frequencies are identical constitute a basis or a representation of the whole group of the crystal. For his reason it is possible to draw some conclusions about the ormal vibrations from the properties of the group and its rreducible representations.

THE GROUP OF A CUBIC CRYSTAL

In discussing the properties of this group I shall go into onsiderable detail in giving illustrations which have been nstructive to me. To those who are well versed in group heory these things may seem superfluous, but to me a proof s more convincing when accompanied by an illustration.

The group of translations constitutes an invariant subroup of the whole group. This means that any rotation,

followed by a translation, and then by the inverse of the original rotation, is just equivalent to a simple translation. This invariant sub-group of translations is an Abelian group. All its members commute with one another. It makes no difference in what order they are carried out.

The group of rotations of the crystal is just the group of rotations about its center under which a simple cube is invariant. These are represented in Figure 1 as the transformation of the coordinates x, y, z. The association of these matrices with the rotations of the cube can be seen from the figure. The first element of the group is the identity operation. This leaves everything unchanged. The second element, D_2^1, represents a rotation of 180° about the x-axis. It changes the sign of the y and z coordinates and leaves the x-coordinate unchanged. It is clear from this that a second application of this operation will restore the cube to its original configuration; so the element is of order 2. This is indicated by the subscript. The superscript merely indicates that this is the first of the elements of order 2, and the letter D indicates that it is a pure rotation. The element R_2^1 can be regarded as a rotation about the x-axis of 180° followed by the change in sign of all three coordinates, or the reflection through the origin. This is the justification for the notation. The element $R_2^1 = JD_2^1$. A simpler view of this element is that it is a reflection in the y-z-plane.

As another example take the element D_3^2. This is a rotation through an angle $2\pi/3$ about the axis symmetrically between x, y, and z. By this operation $x' = z, y' = x, z' = y$. This is obviously an operation of order 3. (There are also operations of order 4 which consist of rotations through 90° about axes parallel to the coordinate axes.)

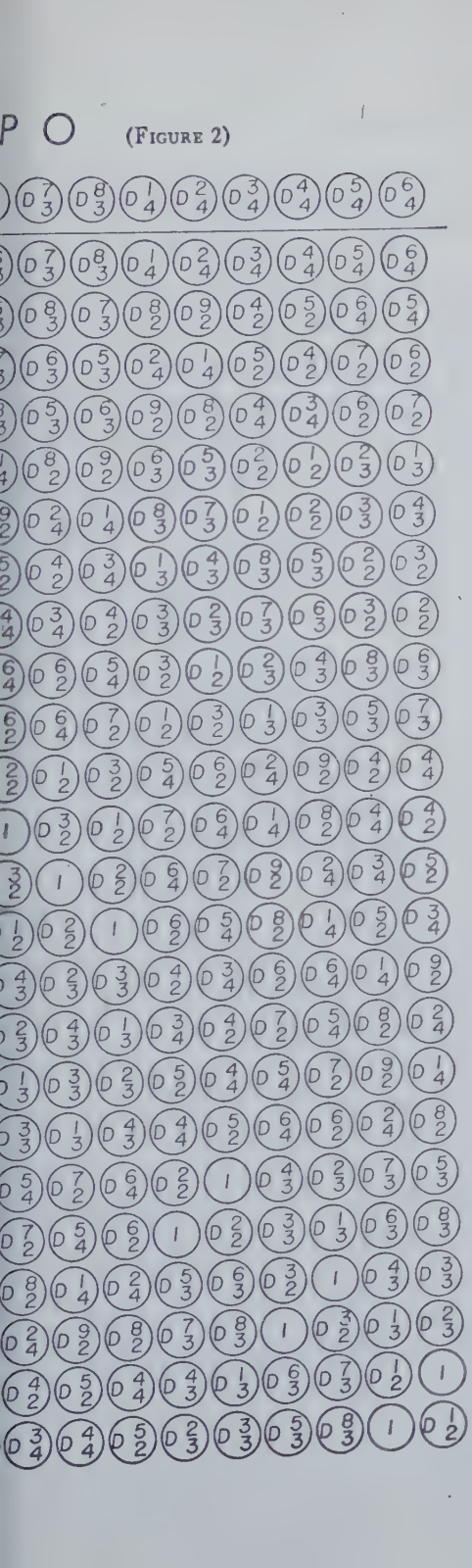
The 24 elements which represent pure rotations constitute an invariant sub-group of the whole. When this invariant

FIGURE 1

MULTIPLICATION TA GRO

1	$\frac{1}{2}$	$\frac{2}{2}$	$\frac{3}{2}$	$\frac{4}{2}$	$\frac{5}{2}$	$\frac{6}{2}$	$\frac{7}{2}$	$\frac{8}{2}$	$\frac{9}{2}$		$\frac{3}{3}$	$\frac{5}{3}$	
$\frac{1}{2}$	1	$\frac{3}{2}$	$\frac{2}{2}$	$\frac{3}{4}$	$\frac{4}{4}$	$\frac{7}{2}$	$\frac{6}{2}$	$\frac{1}{4}$	$\frac{2}{4}$		$\frac{2}{3}$	$\frac{6}{3}$	
$\frac{2}{2}$	$\frac{3}{2}$	1	$\frac{1}{2}$	$\frac{4}{4}$	$\frac{3}{4}$	$\frac{6}{4}$	$\frac{5}{4}$	$\frac{9}{2}$	$\frac{8}{2}$		$\frac{3}{3}$	$\frac{8}{3}$	
$\frac{3}{2}$	$\frac{2}{2}$	$\frac{1}{2}$	1	$\frac{5}{2}$	$\frac{4}{2}$	$\frac{5}{4}$	$\frac{6}{4}$	$\frac{2}{4}$	$\frac{1}{4}$		$\frac{1}{3}$	$\frac{7}{3}$	
$\frac{4}{2}$	$\frac{4}{4}$	$\frac{3}{4}$	$\frac{5}{2}$	1	$\frac{3}{2}$	$\frac{3}{3}$	$\frac{4}{3}$	$\frac{7}{3}$	$\frac{8}{3}$		$\frac{7}{2}$	$\frac{2}{4}$	
$\frac{5}{2}$	$\frac{3}{4}$	$\frac{4}{4}$	$\frac{4}{2}$	$\frac{3}{2}$	1	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{5}{3}$	$\frac{6}{3}$		$\frac{6}{4}$	$\frac{8}{2}$	
$\frac{6}{2}$	$\frac{7}{2}$	$\frac{5}{4}$	$\frac{6}{4}$	$\frac{7}{3}$	$\frac{6}{3}$	1	$\frac{1}{2}$	$\frac{3}{3}$	$\frac{2}{3}$		$\frac{2}{4}$	$\frac{4}{4}$	
$\frac{7}{2}$	$\frac{6}{2}$	$\frac{6}{4}$	$\frac{5}{4}$	$\frac{8}{3}$	$\frac{5}{3}$	$\frac{1}{2}$	1	$\frac{1}{3}$	$\frac{4}{3}$		$\frac{9}{2}$	$\frac{5}{2}$	
$\frac{8}{2}$	$\frac{2}{4}$	$\frac{9}{2}$	$\frac{1}{4}$	$\frac{3}{3}$	$\frac{1}{3}$	$\frac{7}{3}$	$\frac{5}{3}$	1	$\frac{2}{2}$		$\frac{5}{2}$	$\frac{4}{4}$	$\frac{7}{2}$
$\frac{9}{2}$	$\frac{1}{4}$	$\frac{8}{2}$	$\frac{2}{4}$	$\frac{4}{3}$	$\frac{2}{3}$	$\frac{6}{3}$	$\frac{8}{3}$	$\frac{2}{2}$	1		$\frac{3}{4}$	$\frac{4}{2}$	$\frac{5}{2}$
$\frac{1}{3}$	$\frac{2}{3}$	$\frac{4}{3}$	$\frac{3}{3}$	$\frac{1}{4}$	$\frac{8}{2}$	$\frac{3}{4}$	$\frac{5}{2}$	$\frac{7}{2}$	$\frac{6}{4}$	$\frac{5}{3}$		$\frac{6}{3}$	1
$\frac{2}{3}$	$\frac{1}{3}$	$\frac{3}{3}$	$\frac{4}{3}$	$\frac{2}{4}$	$\frac{9}{2}$	$\frac{5}{2}$	$\frac{3}{4}$	$\frac{5}{4}$	$\frac{6}{2}$	$\frac{8}{3}$		$\frac{7}{3}$	
$\frac{3}{3}$	$\frac{4}{3}$	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{8}{2}$	$\frac{1}{4}$	$\frac{4}{2}$	$\frac{4}{4}$	$\frac{6}{2}$	$\frac{5}{4}$	$\frac{6}{3}$		$\frac{5}{3}$	
$\frac{4}{3}$	$\frac{3}{3}$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{9}{2}$	$\frac{2}{4}$	$\frac{4}{4}$	$\frac{2}{4}$	$\frac{6}{4}$	$\frac{7}{2}$	$\frac{7}{3}$		$\frac{8}{3}$	
$\frac{5}{3}$	$\frac{7}{3}$	$\frac{6}{3}$	$\frac{8}{3}$	$\frac{5}{4}$	$\frac{7}{2}$	$\frac{2}{4}$	$\frac{8}{2}$	$\frac{5}{2}$	$\frac{4}{4}$	1		$\frac{2}{2}$	
$\frac{6}{3}$	$\frac{8}{3}$	$\frac{5}{3}$	$\frac{7}{3}$	$\frac{6}{4}$	$\frac{6}{2}$	$\frac{9}{2}$	$\frac{1}{4}$	$\frac{4}{4}$	$\frac{5}{2}$	$\frac{1}{2}$		$\frac{3}{2}$	
$\frac{7}{3}$	$\frac{5}{3}$	$\frac{8}{3}$	$\frac{6}{3}$	$\frac{6}{2}$	$\frac{6}{4}$	$\frac{8}{2}$	$\frac{2}{4}$	$\frac{4}{2}$	$\frac{3}{4}$	$\frac{3}{2}$		$\frac{1}{2}$	
$\frac{8}{3}$	$\frac{6}{3}$	$\frac{7}{3}$	$\frac{5}{3}$	$\frac{7}{2}$	$\frac{5}{4}$	$\frac{1}{4}$	$\frac{9}{2}$	$\frac{3}{4}$	$\frac{4}{2}$	$\frac{2}{2}$		1	
$\frac{1}{4}$	$\frac{9}{2}$	$\frac{2}{4}$	$\frac{8}{2}$	$\frac{1}{3}$	$\frac{3}{3}$	$\frac{8}{3}$	$\frac{6}{3}$	$\frac{1}{2}$	$\frac{3}{2}$	$\frac{4}{4}$		$\frac{5}{2}$	
$\frac{2}{4}$	$\frac{8}{2}$	$\frac{1}{4}$	$\frac{9}{2}$	$\frac{2}{3}$	$\frac{4}{3}$	$\frac{5}{3}$	$\frac{7}{3}$	$\frac{3}{2}$	$\frac{1}{2}$	$\frac{4}{2}$		$\frac{3}{4}$	
$\frac{3}{4}$	$\frac{5}{2}$	$\frac{4}{2}$	$\frac{4}{4}$	$\frac{1}{2}$	$\frac{2}{2}$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{8}{3}$	$\frac{7}{3}$	$\frac{5}{4}$		$\frac{6}{2}$	
$\frac{4}{4}$	$\frac{4}{2}$	$\frac{5}{2}$	$\frac{3}{4}$	$\frac{2}{2}$	$\frac{1}{2}$	$\frac{4}{3}$	$\frac{3}{3}$	$\frac{6}{3}$	$\frac{5}{3}$	$\frac{6}{2}$		$\frac{5}{4}$	
$\frac{5}{4}$	$\frac{6}{4}$	$\frac{6}{2}$	$\frac{7}{2}$	$\frac{5}{3}$	$\frac{8}{3}$	$\frac{3}{2}$	$\frac{2}{2}$	$\frac{2}{3}$	$\frac{3}{3}$	$\frac{9}{2}$		$\frac{8}{2}$	
$\frac{6}{4}$	$\frac{5}{4}$	$\frac{7}{2}$	$\frac{6}{2}$	$\frac{6}{3}$	$\frac{7}{3}$	$\frac{2}{2}$	$\frac{3}{2}$	$\frac{4}{3}$	$\frac{1}{3}$	$\frac{2}{4}$		$\frac{1}{4}$	

P O (FIGURE 2)



sub-group is augmented by the element J, the inversion through the origin, there results the complete group O^h of 48 elements.

The properties of a group are all given by its multiplication table. Figure 2 gives the multiplication table for the group O. This is, of course, just 1/4 of the table for the whole group but the rest can be easily inferred from that much. This table is the real definition of the group. The association of the elements with the rotation of a cube, or with the transformation of coordinates, is merely a representation or an illustration of the group. Nevertheless, it is the representations that are of interest in applications to physics.

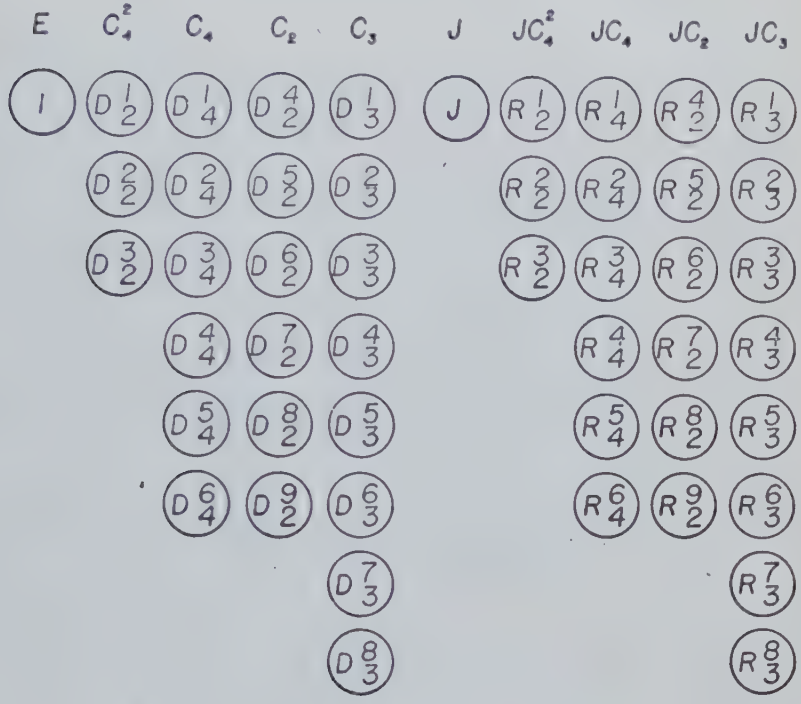
Figure 3 shows some of the properties of this group based entirely on its multiplication table. There is first the division into classes. If an element A is multiplied on the right by another element B and on the left by the inverse of B, the result is another element in the same class. Such a process is called the transformation of the element A by the element B. The transformation of any element A of a group by any other element of the group leads to an element which belongs to the same class as A. Thus the transformation of the element D_4^2 by D_2^6 leads to D_4^4, which is a member of the class C_4 as was D_4^2.

Any group of elements which constitutes a group by itself is called a sub-group. The unit element is a sub-group, but a trivial one. The unit element and the element D_2^1 constitute a sub-group whose multiplication table is given in the figure. An invariant sub-group is a sub-group which contains only whole classes. Every member of an invariant sub-group is transformed into another member of the sub-group by any element of the whole group. The group composed of the unit element and D_2^1 is a sub-group, but it is not an

ariant sub-group since it contains only one of the ele-
nts of the class C_4^2 and that element, D_2^1, is transformed
o D_2^3 by D_3^1. The group G is the smallest invariant sub-
up larger than the identity element itself. The next larger
ariant sub-group is T, which is composed of G and the
ments of the class C_3. It can also be constructed by multi-
ing each element of the sub-group G by D_3^1 and then
$)^2$. The group T contains three times as many elements
the group G.

t is also possible to regard the operation of multiplying
h element of the sub-group G by D_3^1 as a group operation.
it is called A and its square B, the multiplication table
hown in the figure. Such a group is called a factor group,
d is designated by $\frac{T}{G}$. At the bottom of the figure is shown
composition series of O^h. O is the largest invariant sub-
up in O^h. The whole group O^h can be obtained from O
adding $O \times J$. The factor group $\frac{O^h}{O}$ has just two elements;
it is of the order 2. T is the largest invariant sub-group
O and $\frac{O}{T}$ is also of the order 2. Similarly G is the largest
ariant sub-group in T and, as shown, $\frac{T}{G}$ is of the order 3.
is the largest invariant sub-group of G. One should note
at F is an invariant sub-group of G, but is not an invariant
-group of the whole group O^h. Transformation of F by
ments of G leaves it invariant, but transformation of F
elements outside of G but still in the group O^h does not
ve it invariant. The factor group $\frac{G}{F}$ is of order 2 and
ally the factor group $\frac{F}{E}$ is of order 2. Such a series of
ariant sub-groups is called a composition series. When
of the factor groups are of prime order, as in this case,

CLASSES OF THE GROUP O^*



INVARIANT SUBGROUPS OF

$$E$$

$$G = E + C_4^2$$

$$T = G + C_3$$

$$O = T + C_4 + C_2$$

$$O^* = O + JO$$

A COMPOSITION SERIES OF

$$O^*, O, T, G, F, E$$

FIGURE 3

LTIPLICATION TABLES

ROUP F

1	D_2^1
1	D_2^1
D_2^1	1

SUB-GROUP G

1	D_2^1	D_2^2	D_2^3
1	D_2^1	D_2^2	D_2^3
D_2^1	1	D_2^3	D_2^2
D_2^2	D_2^3	1	D_2^1
D_2^3	D_2^2	D_2^1	1

TOR GROUP

$\frac{T}{G}$

E	A	B
E	A	B
A	B	E
B	E	A

AUGMENTATION OF G

BY D_3^1

G	D_3^1G	$D_3^1{}^2$G
1	D_3^1	D_3^5
D_2^1	D_3^2	D_3^7
D_2^2	D_3^4	D_3^6
D_2^3	D_3^3	D_3^8

FIGURE 3 (Cont.)

the whole group, O^h, is said to be resolvable. Seitz has shown that all groups represented by crystals are resolvable. This property of resolvability is of importance in the reduction of the representation.

The set of linear transformations, in terms of which this group of rotations was specified, constitutes a representation of the group. The transformation matrices obey the same laws of multiplication as the group elements. It is possible, however, to construct many other representations. Suppose, for instance, that instead of the coordinates x, y, z one takes all their quadratic combinations x^2, y^2, z^2, xy, xz, yz, and applies to them the transformation indicated in the first representation. The matrices of these transformations will contains six rows and six columns, and will constitute a representation of the group. Some examples of these matrices are given in Figure 4. This shows one representative from each class and in the bottom row are three from the class JC_3.

A common property of all these matrices is that they consist of two 3×3 matrices along the diagonal. The upper right and lower left squares consist entirely of zeros. This fact is described by saying that the representation is partly reduced. If it were possible, by using linear combinations of these quadratic terms instead of the simple products themselves, to reduce all the matrices to smaller square matrices along the diagonal, the representation would be further reducible. As a matter of fact, this representation is reducible. The matrices in the lower right-hand corner cannot be reduced, but those in the upper left corner can be. This is shown in Figure 5. The new variables are

$$R=x^2+y^2+z^2 \quad S=x^2+\epsilon^2y^2+\epsilon z^2 \quad T=x^2+\epsilon y^2+\epsilon^2z^2$$

and each of the matrices consists of one single term and a

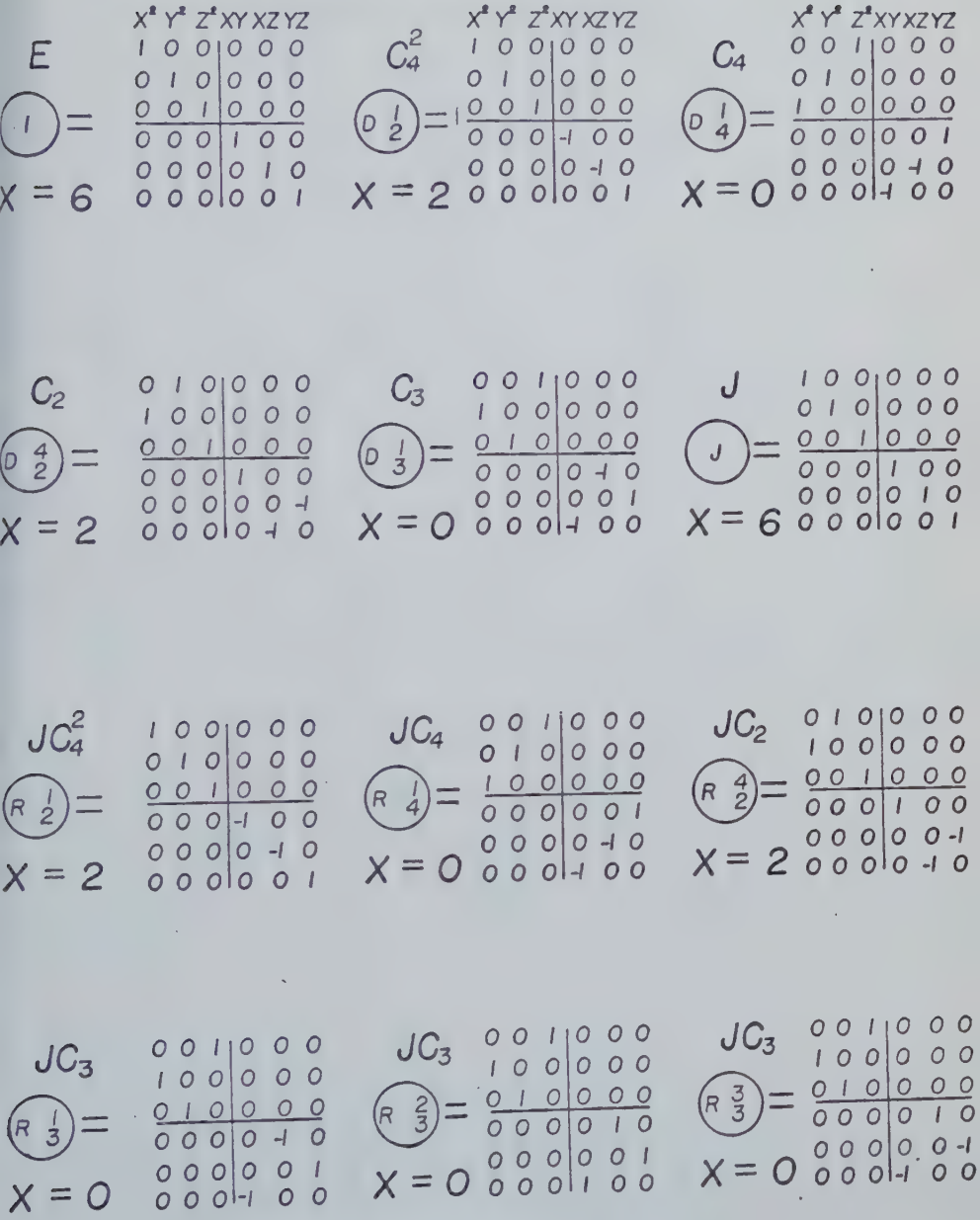


FIGURE 4—A REPRESENTATION OF GROUP O^h

A REDUCED REPRESENTATION OF O^h

LET $R = X^2 + Y^2 + Z^2$

$S = X^2 + \epsilon^2 Y^2 + \epsilon Z^2$

$T = X^2 + \epsilon Y^2 + \epsilon^2 Z^2$ $\qquad \epsilon = 1^{\frac{1}{3}}$

E	C_4^2	C_4^2	C_4
$(1) =$	$(D\,\frac{1}{2}) =$	$(D\,\frac{2}{2}) =$	$(D\,\frac{1}{4}) =$
R S T 1 | 0 0 0 | 1 0 0 | 0 1	R S T 1 | 0 0 0 | 1 0 0 | 0 1	R S T 1 | 0 0 0 | 1 0 0 | 0 1	R S T 1 | 0 0 0 | 0 ϵ 0 | ϵ^2 0
$X = 3$	$X = 3$	$X = 3$	$X = 1$

C_4	C_2	C_3	C_3
$(D\,\frac{6}{4}) =$	$(D\,\frac{4}{2}) =$	$(D\,\frac{1}{3}) =$	$(D\,\frac{2}{3}) =$
1 | 0 0 0 | 0 1 0 | 1 0	1 | 0 0 0 | 0 ϵ^2 0 | ϵ 0	1 | 0 0 0 | ϵ 0 0 | 0 ϵ^2	1 | 0 0 0 | ϵ 0 0 | 0 ϵ^2
$X = 1$	$X = 1$	$X = 0$	$X = 0$

J	JC_4^2	JC_4^2	JC_4
$(J) =$	$(R\,\frac{1}{2}) =$	$(R\,\frac{3}{2}) =$	$(R\,\frac{1}{4}) =$
1 | 0 0 0 | 1 0 0 | 0 1	1 | 0 0 0 | 1 0 0 | 0 1	1 | 0 0 0 | 1 0 0 | 0 1	1 | 0 0 0 | 0 ϵ 0 | ϵ^2 0
$X = 3$	$X = 3$	$X = 3$	$X = 1$

JC_4	JC_2	JC_3	JC_3
$(R\,\frac{5}{4}) =$	$(R\,\frac{4}{2}) =$	$(R\,\frac{1}{3}) =$	$(R\,\frac{3}{3}) =$
1 | 0 0 0 | 0 1 0 | 1 0	1 | 0 0 0 | 0 ϵ^2 0 | ϵ 0	1 | 0 0 0 | ϵ 0 0 | 0 ϵ^2	1 | 0 0 0 | ϵ 0 0 | 0 ϵ^2
$X = 1$	$X = 1$	$X = 0$	$X = 0$

FIGURE 5

2 matrix on the diagonal. In this way the original rep-
entation containing six rows and six columns can be con-
ered as composed of a one-dimensional, a two-dimen-
nal, and a three-dimensional irreducible representation.
is is the limit of possible reduction in this case.

Each group has a set of irreducible representations. For a
ite group, the number of such representations is finite.
ur of the irreducible representations of this group O^h have
en already shown. The original matrices constitute one,
d the other three are included in the six-row, six-column
atrices just discussed.

An important theorem in the theory of representations
that every representation is composed, in a unique way,
irreducible representations. For instance the six-row,
-column representation just discussed has been shown to
composed of one 1-dimensional, one 2-dimensional, and
e 3-dimensional irreducible representation. It might be
rought that this reduction could be carried out in many
fferent ways, but such is not the case. A given representa-
on can be reduced to only one set of irreducible represen-
tions. It is largely because of this theorem that the theory
group representations is useful in treating the equations
physics.

Any representation of a group can be described by means
its group characters. These are the diagonal sums of the
atrices of the representation. This diagonal sum is the
me for all the members of a class, so that it is necessary
give the character merely for each class, and not for each
ement of the group. In the chart showing the six-dimen-
onal representation, the identity matrix has the character
The identity will always have a character equal to the
mber of dimensions of the representation. The class C_4^2
s the character 2 and the other characters are indicated

on the chart. In particular, the three elements of the class JC_3 are all shown to have the same character 0.

When the characters of the representations are given, the representation is essentially defined. Matrix transformations of the form $A^{-1}BA$ lead to what is known as an equivalent representation. Such representations are regarded as not being essentially distinct from the original even though the form of the matrices will be different. Such transformations do not change the characters of the representation. For this reason, new representations which have the same set of characters are either identical or equivalent representations.

Each irreducible representation of a group has a set of group characters which uniquely define it. In the chart showing the identity representation and the two-dimensional representation, it can be seen that all the characters of the identity are 1. In the two-dimensional representation the character of the unit element is naturally 2; for the class C_4^2 the character is also 2, as shown in the two examples. For classes C_4, C_2, JC_4, and JC_2 the character is zero; for class C_3 and class JC_3 it is -1, and for J and JC_4^2 the character is 2. The specification of this set of numbers, together with the classes to which they belong, completely specifies this particular irreducible representation. The characters of the irreducible representations of O^h are shown in Figure 6.

If a representation is composed of a number of irreducible representations, the character of each class is the sum of the characters of the various irreducible representations of the class. Furthermore, the properties of the characters are such that this sum can be made up in one and only one way, corresponding to the unique reduction of the representation. In this way it is possible to determine the irreducible representations of which any representation is composed, provided the characters are known.

CHARACTERS OF THE
IRREDUCIBLE REPRESENTATION
OF THE GROUP O^h

1	3	6	6	8	1	3	6	6	8
E	C_4^2	C_4	C_2	C_3	J	JC_4^2	JC_4	JC_2	JC_3
1	1	1	1	1	1	1	1	1	1
1	1	-1	-1	1	1	1	-1	-1	1
2	2	0	0	-1	2	2	0	0	-1
3	-1	1	-1	0	3	-1	1	-1	0
3	-1	-1	1	0	3	-1	-1	1	0
1	1	1	1	1	-1	-1	-1	-1	-1
1	1	-1	-1	1	-1	-1	1	1	-1
2	2	0	0	-1	-2	-2	0	0	1
3	-1	1	-1	0	-3	1	-1	1	0
3	-1	-1	1	0	-3	1	1	-1	0

FIGURE 6

GROUP REPRESENTATIONS BASED ON THE NORMAL VIBRATIONS

Let us now return to the vibrations of a cubic crystal and attempt to form a representation of the whole group on the basis of them. In the first place, one could use the displacements of the individual lattice points as the basis of such a representation. Each point has three possible components of displacement and there are G^3 points; so the representation would be $3G^3$ dimensional. To start to reduce this representation, consider first the invariant sub-group consisting of the translations alone. Since the group is Abelian it has only one-dimensional irreducible representations; and since every element is of the order G, each matrix must be diagonal with Gth roots of unity on the diagonal. The linear combinations which are the basis for such a reduced representation are

$$\rho_{j,k_1,k_2,k_3} = \sum_{l,m,n} e^{\frac{2\pi i}{G}(k_1 l + k_2 m + k_3 n)} r_{j,l,m,n}$$

A translation of the lattice obviously multiplies each of these quantities by a root of unity, and a G-fold iteration of any translation restores the variables to their original values. This constitutes a completely reduced representation of the invariant sub-group of translations. Each ρ is characterized by an index j which can take on the values 1, 2, 3 representing the three possible directions of displacement along x, y, z, and by the three integers k_1, k_2, k_3. These integers can take on values from $-\frac{G}{2}$ to $+\frac{G}{2}$ and the triplets of integers may be represented by vectors in the k_1, k_2, k_3 space. The ends of the possible vectors fill uniformly a cube of edge G.

If a rotation element of the group O^h is applied to one of these $\rho_{j,k_1k_2k_3}$ it will, in general, transform it to a different k_1', k_2', k_3' and a linear combination of the indices j. Since

he differential equation of motion is invariant to such a otation, the time dependence of the transformed displacement will be the same as that of the original. If such linear ombinations of the indices j are formed as to give a normal oordinate, the rotation will transform it into another normal coordinate, since the relative displacements are unhanged by the rotation. The transformed normal coordiate will also have the same frequency as the original. For general vector $(k_1k_2k_3)$ there are 48 directions in which it

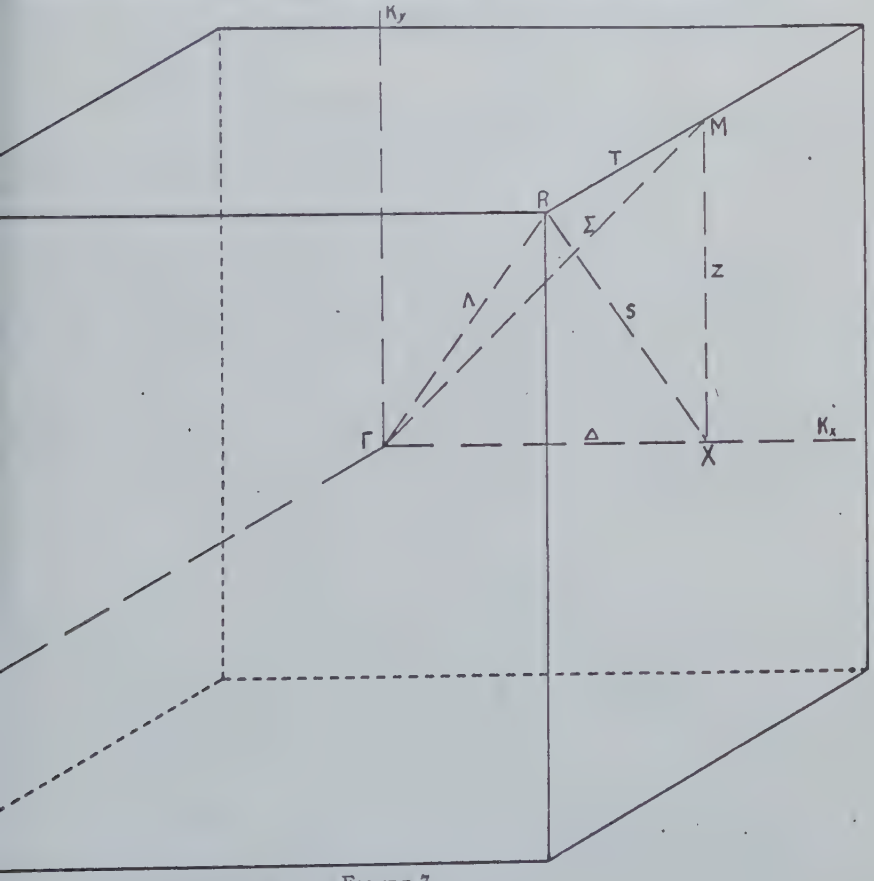


FIGURE 7

can be rotated by the members of the group, and so there are 48 normal vibrations with the same frequency of vibration, and in general there are three frequencies for each value of $k_1k_2k_3$. This, however, gives no direct information about the frequencies or the form of the vibrations, except to show that only 1/48 of the whole cube need be considered in computing them. In special cases, however, some such information can be obtained, and by making use of the fact that the frequencies and the forms of vibration vary continuously with k, it is possible to infer some additional information.

Consider first the case where $k=0$. This is designated by Γ in Figure 7. A transformation of ρ_{j000} by any of the elements of the group O^h leaves the value of k invariant and affects only the index j. The group of the vectors ending at Γ is the whole cubic group. The representation based on these coordinates will be a three-dimensional representation and will be just the representation shown for the description of the operators. It is based on x, y, and z and is an irreducible representation. This means that for $k=0$, vibrations in any direction are normal vibrations and they all have the same frequency. At this point the three possible frequencies of vibration coincide.

Consider next those vectors k for which $k_2=k_3=0$. These terminate along the line Δ in the figure. There is a subgroup of the group of rotation to which these wave vectors are invariant. The elements and properties of this group are shown in Figure 8. The characters of the representation of this sub-group that is based on x, y, z are given in the first row. Then follow the characters of the irreducible representations of Δ and finally the composition of the representation at hand in terms of the irreducible representation. Δ_1 is a one-dimensional representation and is based on ρ_x. This

CHARACTERS OF THE SUB-GROUPS Δ AND S

Δ

ELEMENTS	(1)	$(D\frac{1}{2})$	$(D\frac{3}{4})$	$(R\frac{2}{2})$	$(R\frac{6}{2})$	$(D\frac{5}{4})$	$(R\frac{3}{2})$	$(R\frac{7}{2})$
CLASSES	E	C_4^2	C_4	JC_4^2	JC_2			
Δ	3	-1	1	1	1			
Δ_1	1	1	1	1	1			
Δ_2	1	1	-1	1	-1			
$\Delta_{2'}$	1	1	-1	-1	1			
$\Delta_{1'}$	1	1	1	-1	-1			
Δ_5	2	-2	0	0	0			

$\Delta = \Delta_1 + \Delta_5$

Δ_1 IS BASED ON P_x

Δ_5 IS BASED ON P_y AND P_z

S

ELEMENTS	(1)	$(D\frac{7}{2})$	$(R\frac{1}{2})$	$(R\frac{5}{2})$
CLASSES	E	C_2	JC_4^2	JC_2
S	3	-1	1	1
S_1	1	1	1	1
S_2	1	1	-1	-1
S_3	1	-1	-1	1
S_4	1	-1	1	-1

$S = S_1 + S_3 + S_4$

S_1 IS BASED ON $P_y + P_z$

S_3 IS BASED ON P_x

S_4 IS BASED ON $P_y - P_z$

FIGURE 8

means that a vibration along the x-axis is a normal vibration with a frequency characteristic of it. Δ_5 is a two-dimensional representation based on ρ_y and ρ_z. Any linear combination of ρ_y and ρ_z is a normal vibration, and the two independent linear combinations have the same frequency. A similar consideration of the group to which the vectors ending at X is invariant shows that at X there are still only two independent frequencies. All along the line Δ the vibrations have the nature of transverse and longitudinal waves as in an elastic continuum, and there are two independent frequencies.

Again the vectors that end along the line S are invariant to a sub-group S whose properties are shown. This sub-group can be completely reduced as shown, and the reduced

TWO HOLOMORPHIC SUB-GROUPS OF O^h

GROUP OF T

	1	$D\frac{3}{2}$	$D\frac{3}{4}$	$D\frac{4}{4}$	$R\frac{1}{2}$	$R\frac{2}{2}$	$R\frac{4}{2}$	$R\frac{5}{2}$
1	1	$D\frac{3}{2}$	$D\frac{3}{4}$	$D\frac{4}{4}$	$R\frac{1}{2}$	$R\frac{2}{2}$	$R\frac{4}{2}$	$R\frac{5}{2}$
$D\frac{3}{2}$	$D\frac{3}{2}$	1	$D\frac{4}{4}$	$D\frac{3}{4}$	$R\frac{2}{2}$	$R\frac{1}{2}$	$R\frac{5}{2}$	$R\frac{4}{2}$
$D\frac{3}{4}$	$D\frac{3}{4}$	$D\frac{4}{4}$	$D\frac{3}{2}$	1	$R\frac{5}{2}$	$R\frac{4}{2}$	$R\frac{1}{2}$	$R\frac{2}{2}$
$D\frac{4}{4}$	$D\frac{4}{4}$	$D\frac{3}{4}$	1	$D\frac{3}{2}$	$R\frac{4}{2}$	$R\frac{5}{2}$	$R\frac{2}{2}$	$R\frac{1}{2}$
$R\frac{1}{2}$	$R\frac{1}{2}$	$R\frac{2}{2}$	$R\frac{4}{2}$	$R\frac{5}{2}$	1	$D\frac{3}{2}$	$D\frac{3}{4}$	$D\frac{4}{4}$
$R\frac{2}{2}$	$R\frac{2}{2}$	$R\frac{1}{2}$	$R\frac{5}{2}$	$R\frac{4}{2}$	$D\frac{3}{2}$	1	$D\frac{4}{4}$	$D\frac{3}{4}$
$R\frac{4}{2}$	$R\frac{4}{2}$	$R\frac{5}{2}$	$R\frac{2}{2}$	$R\frac{1}{2}$	$D\frac{4}{4}$	$D\frac{3}{4}$	1	$D\frac{3}{2}$
$R\frac{5}{2}$	$R\frac{5}{2}$	$R\frac{4}{2}$	$R\frac{1}{2}$	$R\frac{2}{2}$	$D\frac{3}{4}$	$D\frac{4}{4}$	$D\frac{3}{2}$	1

CLASSES OF

E	C_4^2	C_4	JC_2
1	$D\frac{3}{2}$	$D\frac{3}{4}$	$R\frac{4}{2}$
		$D\frac{4}{4}$	$R\frac{5}{2}$

GROUP OF Δ

	1	$D\frac{1}{2}$	$D\frac{5}{4}$	$D\frac{6}{4}$	$R\frac{2}{2}$	$R\frac{3}{2}$	$R\frac{7}{2}$	$R\frac{6}{2}$
1	1	$D\frac{1}{2}$	$D\frac{5}{4}$	$D\frac{6}{4}$	$R\frac{2}{2}$	$R\frac{3}{2}$	$R\frac{7}{2}$	$R\frac{6}{2}$
$D\frac{1}{2}$	$D\frac{1}{2}$	1	$D\frac{6}{4}$	$D\frac{5}{4}$	$R\frac{3}{2}$	$R\frac{2}{2}$	$R\frac{6}{2}$	$R\frac{7}{2}$
$D\frac{5}{4}$	$D\frac{5}{4}$	$D\frac{6}{4}$	$D\frac{1}{2}$	1	$R\frac{6}{2}$	$R\frac{7}{2}$	$R\frac{2}{2}$	$R\frac{3}{2}$
$D\frac{6}{4}$	$D\frac{6}{4}$	$D\frac{5}{4}$	1	$D\frac{1}{2}$	$R\frac{7}{2}$	$R\frac{6}{2}$	$R\frac{3}{2}$	$R\frac{2}{2}$
$R\frac{2}{2}$	$R\frac{2}{2}$	$R\frac{3}{2}$	$R\frac{7}{2}$	$R\frac{6}{2}$	1	$D\frac{1}{2}$	$D\frac{5}{4}$	$D\frac{6}{4}$
$R\frac{3}{2}$	$R\frac{3}{2}$	$R\frac{2}{2}$	$R\frac{6}{2}$	$R\frac{7}{2}$	$D\frac{1}{2}$	1	$D\frac{6}{4}$	$D\frac{5}{4}$
$R\frac{7}{2}$	$R\frac{7}{2}$	$R\frac{6}{2}$	$R\frac{3}{2}$	$R\frac{2}{2}$	$D\frac{6}{4}$	$D\frac{5}{4}$	1	$D\frac{1}{2}$
$R\frac{6}{2}$	$R\frac{6}{2}$	$R\frac{7}{2}$	$R\frac{2}{2}$	$R\frac{3}{2}$	$D\frac{5}{4}$	$D\frac{6}{4}$	$D\frac{1}{2}$	1

CLASSES OF

E	C_4^2	C_4	JC_4^2
1	$D\frac{1}{2}$	$D\frac{5}{4}$	$R\frac{2}{2}$
		$D\frac{6}{4}$	$R\frac{3}{2}$

FIGURE 9

presentations are based on $\rho_y+\rho_z$, ρ_x, $\rho_y-\rho_z$. There are hus three different frequencies. In this case there are no ngitudinal or transverse vibrations, but the normal vibra- ons are in the face of the cube and in the x-direction.

The vector ending at the point R is invariant to all mem- ers of the rotation group O^h, and so just as at Γ there is ut one frequency. All of the three possible vibrations at his point have the same frequency. Lines Δ and T have olomorphic groups (Figure 9).

Whenever it is possible to find a wave vector k whose group ontains more than the identity, it is possible to solve the ubic equation which determines the frequencies of vibra- ion. Thus over the surfaces of the portion of the k cube hat it is necessary to consider, the application of the theory f group representations indicates the method of treating he cubic equation and provides a basis for classification of he roots. In case the representation can be completely re- uced, the group theory itself gives the solution of the cubic quation. In cases in which there is still a two-dimensional epresentation left, the theory of group representation gives ne root and the remaining quadratic equation can be easily andled by ordinary methods. For those points inside of his region, some estimate of the frequencies can be obtained y extrapolation from the surface.

This example which I have developed in some detail is, n itself, not very important. There exists no crystal with imple cubic symmetry and the results for such a crystal ould be obtained by more direct, if less elegant, means. Iowever, I think it serves best to illustrate a method which an be applied to crystals of all types and permits an imme- iate recognition of those properties of the elastic spectrum hich are to be attributed to the symmetry of the crystal lone, and are independent of the nature of the forces.

W. V. Houston.